Further developments on emulators for quantum continuum states

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ESNT Workshop: Eigenvector continuation and related techniques in nuclear structure and reaction theory, CEA Saclay, France, May 30, 2023

Outline

- Introduction
- Emulators for continuum states at given real energies
- Emulators for continuum states in energy’s complex plane
- Summary

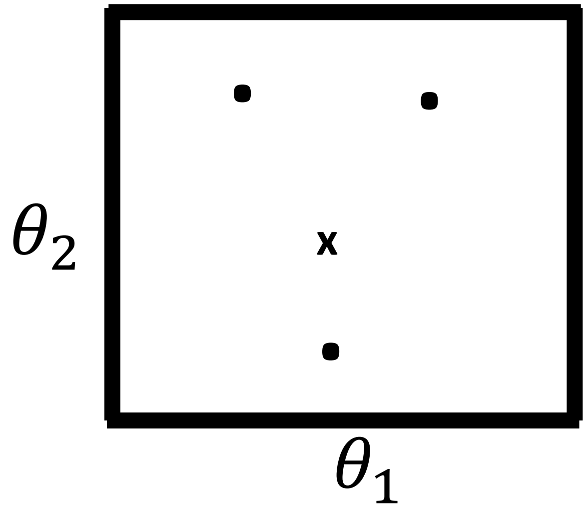
Emulators

Fast and accurate interpolations and extrapolations of inputs vs outputs

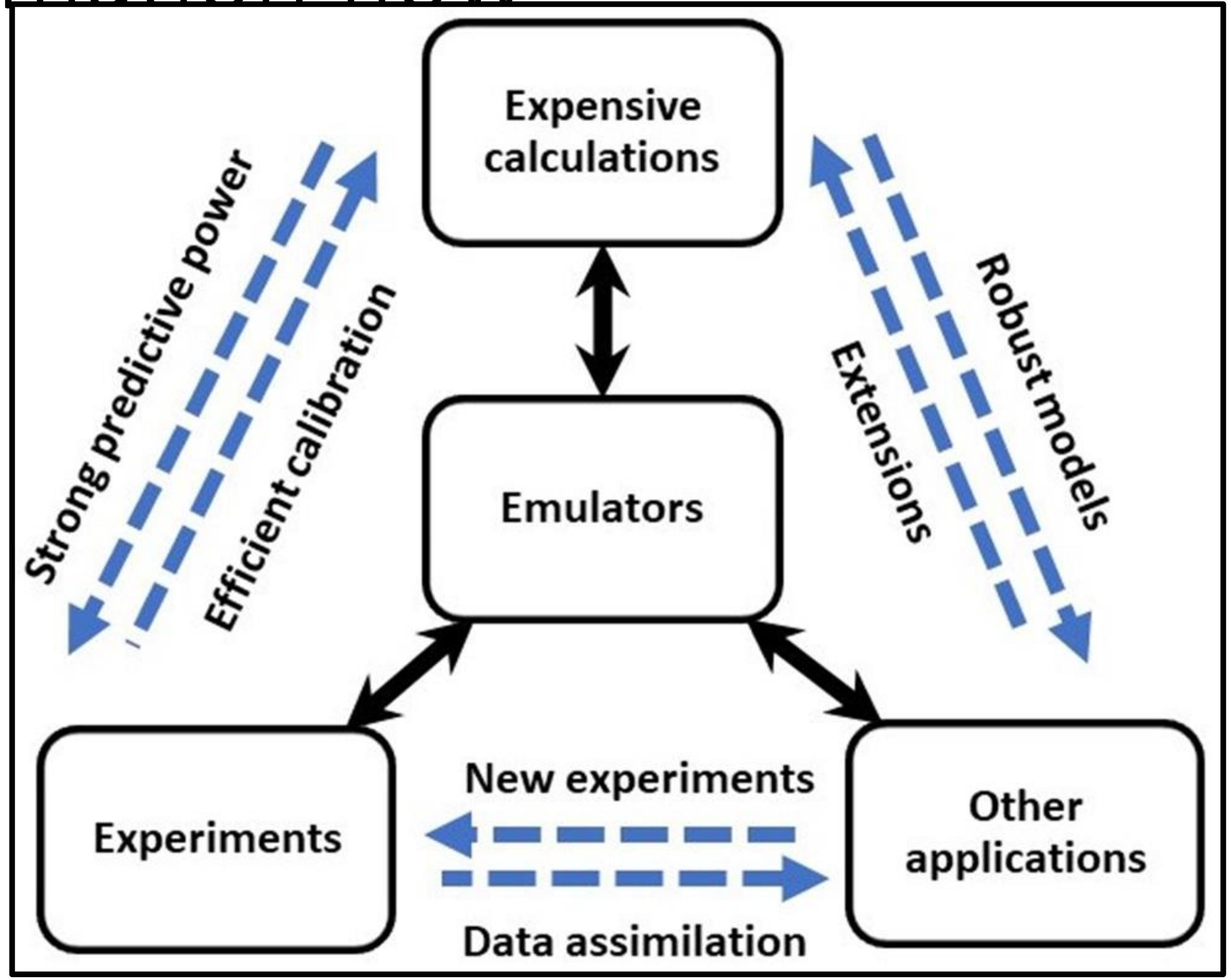
- Model calibrations and error propagations (e.g., UQ in Bayesian statistics)
  - Bound states
  - Continuum states:
    N-d scatterings (three-body force); nuclear reactions

- New calculations
  - Theory matching: macroscopic theories against microscopic calculations
  - Extrapolations from feasible calculations into infeasible regions

Parameter space ($\boldsymbol{\theta}$)



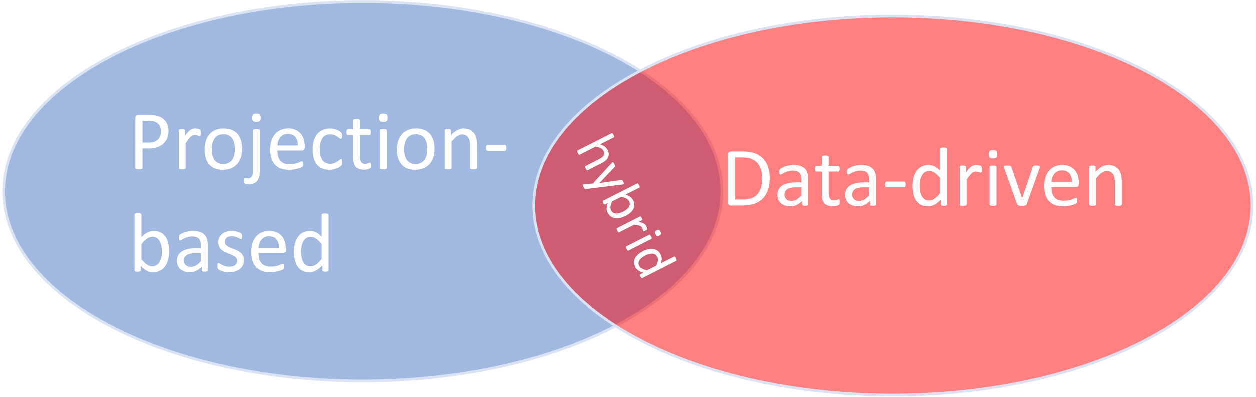
Potential impact on research workflows/information flow



"Fast emulation of quantum **three-body** scattering",
XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022),
[2110.04269](2110.04269)

Emulators

"Eigenvector continuation with subspace learning"
Dillon Frame et. al., *Phys.Rev.Lett.* 121 (2018) 3, 032501, 1711.07090



$$\boldsymbol{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{N_b} C_i(\boldsymbol{\theta})\, \boldsymbol{\psi}(\boldsymbol{\theta}_i)$$

- Reduced basis method/eigenvector continuation (RBM/EC) emulators
- They are Intrusive
- But include more physics, require less training data, and have better extrapolation

- Machine learning (ML): Gaussian process and neural networks
- nonintrusive
- agnostic of physics and requiring more training data

"BUQEYE Guide to Projection-Based Emulators in Nuclear Physics," C. Drischler, J.A. Melendez, R.J. Furnstahl, A.J. Garcia, and XZ, 2212.04912
"Training and projecting: A reduced basis method emulator for many-body physics," Edgard Bonilla, Pablo Giuliani, Kyle Godbey, Dean Lee, *Phys.Rev.C* 106 (2022) 5, 054322, 2203.05284
"Model reduction methods for nuclear emulators, " J.A. Melendez, C. Drischler, R.J. Furnstahl, A.J. Garcia, XZ, 2203.05528

Emulating continuum states at given Es

RBM/EC emulators for continuum states

$$[E - H(\boldsymbol{\theta})]|\psi(\boldsymbol{\theta})\rangle = 0 \ \text{ for a given } E$$

"Efficient emulators for scattering using eigenvector continuation," R. J. Furnstahl, A. J. Garcia, P. J. Millican, and XZ, PLB **809,** 135719 (2020) [2007.03635]

$$\boldsymbol{\psi}(\boldsymbol{\theta}) = \sum_{i=1}^{N_b} C_i(\boldsymbol{\theta})\, \boldsymbol{\psi}(\boldsymbol{\theta}_i)$$

D. Bai & Z. Ren (2021); C. Drischler, et. al., (2021); J.A. Melende et.al., (2021); D. Bai (2022); A.J. Garcia, et.al., (2023)

- RBM/EC emulators for two-body scatterings based on **Kohn** scattering variational principles
- With Coulomb interaction
- Complex optical potential
- General partial waves (or without pw decomp.)
- Emulators without wave functions
- Mitigating Kohn anomalous singularities
- Two-body coupled-channel scatterings

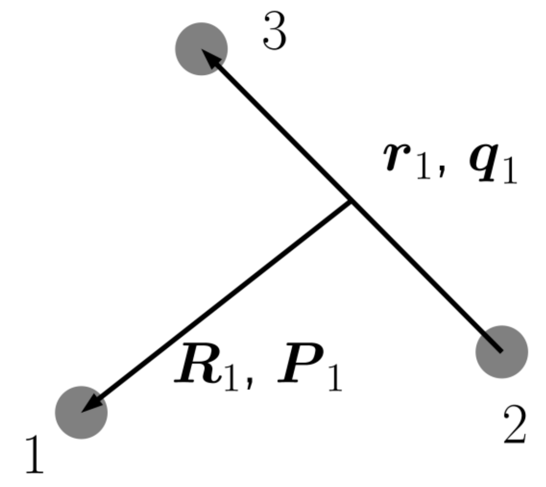
$$\sum_j (\Delta U^T + \Delta U)_{ij} C_j = \tau(\delta_i) - \lambda$$

$$\sum_j C_j = 1$$

$$\Delta U_{ij} \propto \langle \psi(\boldsymbol{\theta_i})|\, 2\, V(\boldsymbol{\theta}) - V_i - V_j |\psi(\boldsymbol{\theta_j})\rangle$$

Affine/factorized structure→ fast emulations

Three-body scattering: below breakup threshold (S wave)



For three identical spin-0 bosons, $H = T_r + T_R + V_{2-body} + V_{3-body}$

Suppose V_{2-body} gives a two-body (dimer) bound state ϕ_b

Compute the boson-dimer scattering. The scattering WF

$$\Psi(\boldsymbol{r_1}, \boldsymbol{R_1}) \xrightarrow{R_1\to\infty} \phi_b(\boldsymbol{r_1}) \frac{1}{\sqrt{v}} [-e^{-iP_1R_1} + S\, e^{iP_1R_1}]$$

The functional estimates the scattering S-matrix:

$$F[\Psi_{\text{trial}}] = S_{\text{trial}} - \frac{1}{3i} \langle \Psi_{\text{trial}} | \widehat{H}(\boldsymbol{\theta}) - E | \Psi_{\text{trial}} \rangle$$

Separable V_{2-body}, e.g., $V_{23} = \lambda |g\rangle\langle g|$

$$\langle \boldsymbol{q_1} | g \rangle \propto e^{-q_1^2/(2\Lambda^2)}$$

Separable V_{3-body}: $V_4 = \lambda_4 |g_4\rangle\langle g_4|$

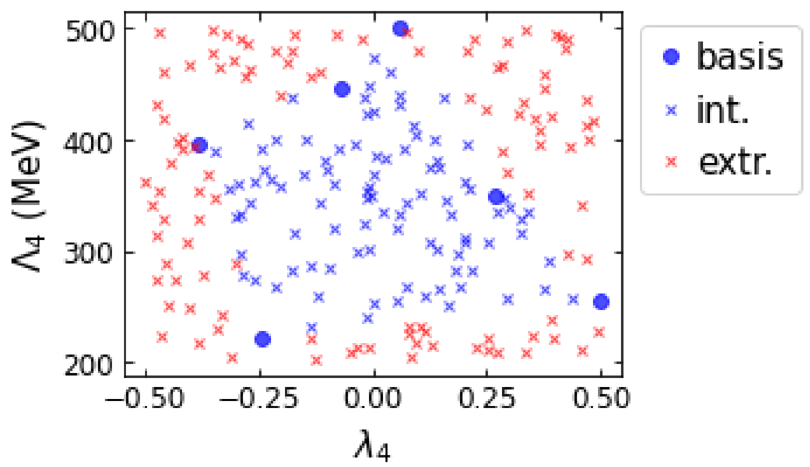
$$\langle \boldsymbol{P_1 q_1} | g_4 \rangle \propto e^{-(q_1^2 + \frac{3}{4}P_1^2)/(2\Lambda_4^2)}$$

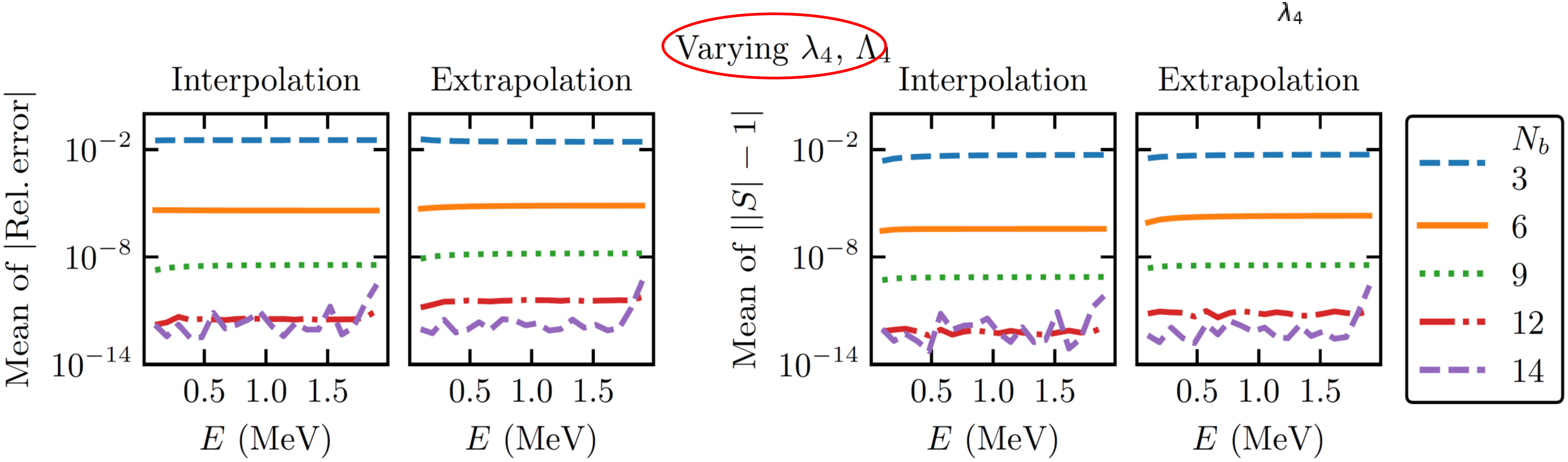
Mass as nucleon mass

"Fast emulation of quantum **three-body** scattering",
XZ and R.J. Furnstahl, Phys. Rev. C 105, 064004 (2022), 2110.04269

Accuracy

blue crosses: interpolation
red ones: extrapolations

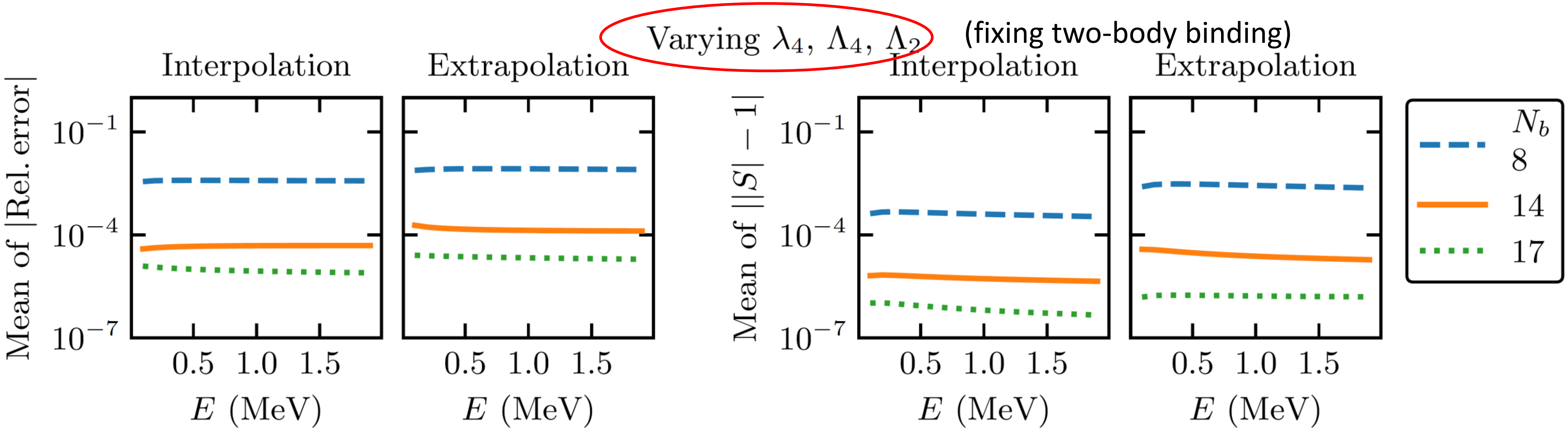




- $\Lambda_4 \in [200, 500]$ MeV
- $\lambda_4 \in [-0.5, 0.5]$

Accuracy

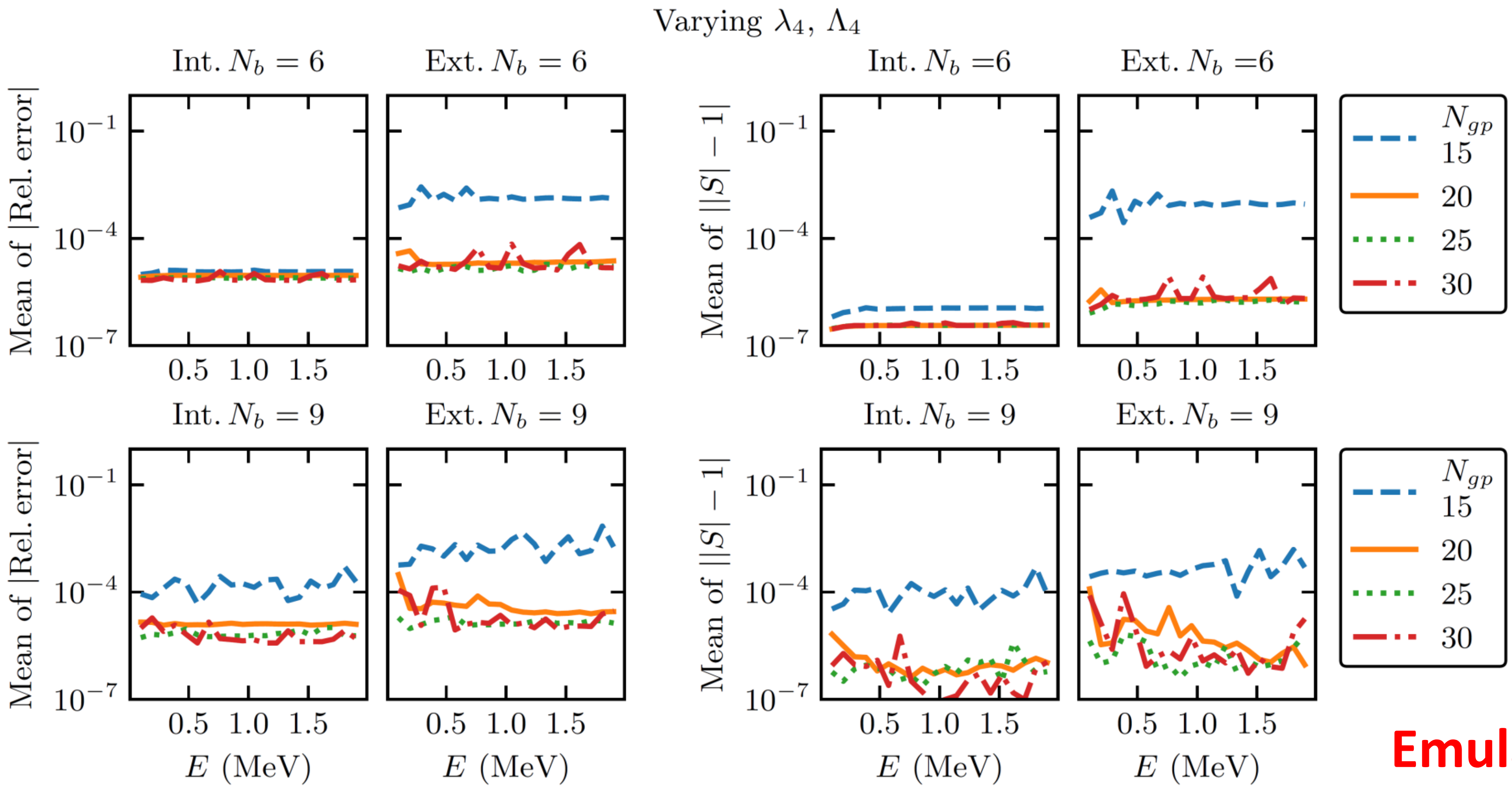
Difficulty: the training and test pts have different 2-body bound states (i.e., asymptotic behavior)



- $\Lambda_2, \Lambda_4 \in [200, 500]$ MeV
- $\lambda_4 \in [-0.5, 0.5]$

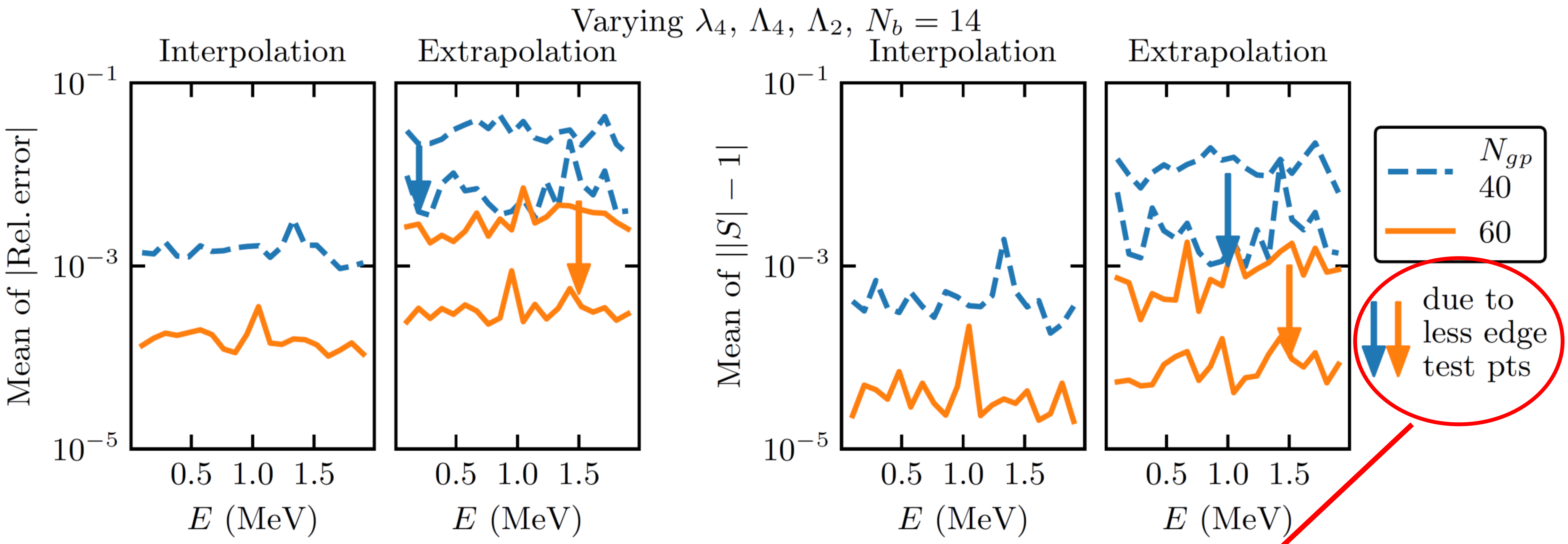
Emulator in emulator

Gaussian Process interpolates $\Delta U(\boldsymbol{\theta})$ in the parameter space



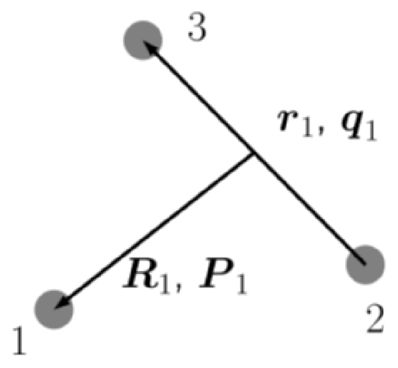
Emulator costs 10^{-3} seconds

Emulator in emulator



For Λ_2, Λ_4, $[200, 500] \rightarrow [230, 470]$ MeV

Performance



EC emulators	S relative error	Time	Memory
linear[a]	10^{-14} to 10^{-13}	ms	< MB
nonlinear-1	10^{-6} to 10^{-5}	ms	MB
nonlinear-2	10^{-4}	ms	10s MB

In contrast, the costs of full realistic calculations are 10^3s

These studies require the same real energy for trainings and emulations.

$$[E - H(\boldsymbol{\theta})]|\psi_{sc}(E,\boldsymbol{\theta})\rangle = |S\rangle$$

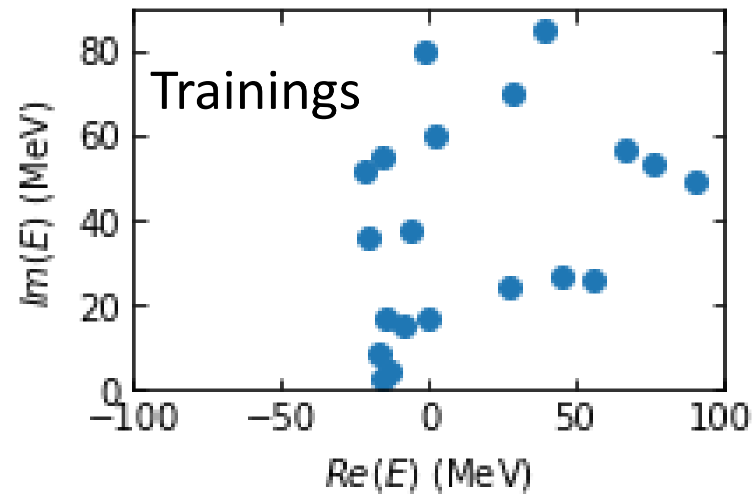
$$\longrightarrow \quad \langle S'|\psi_{sc}(E,\boldsymbol{\theta})\rangle$$

Emulating continuum states in E's complex plane

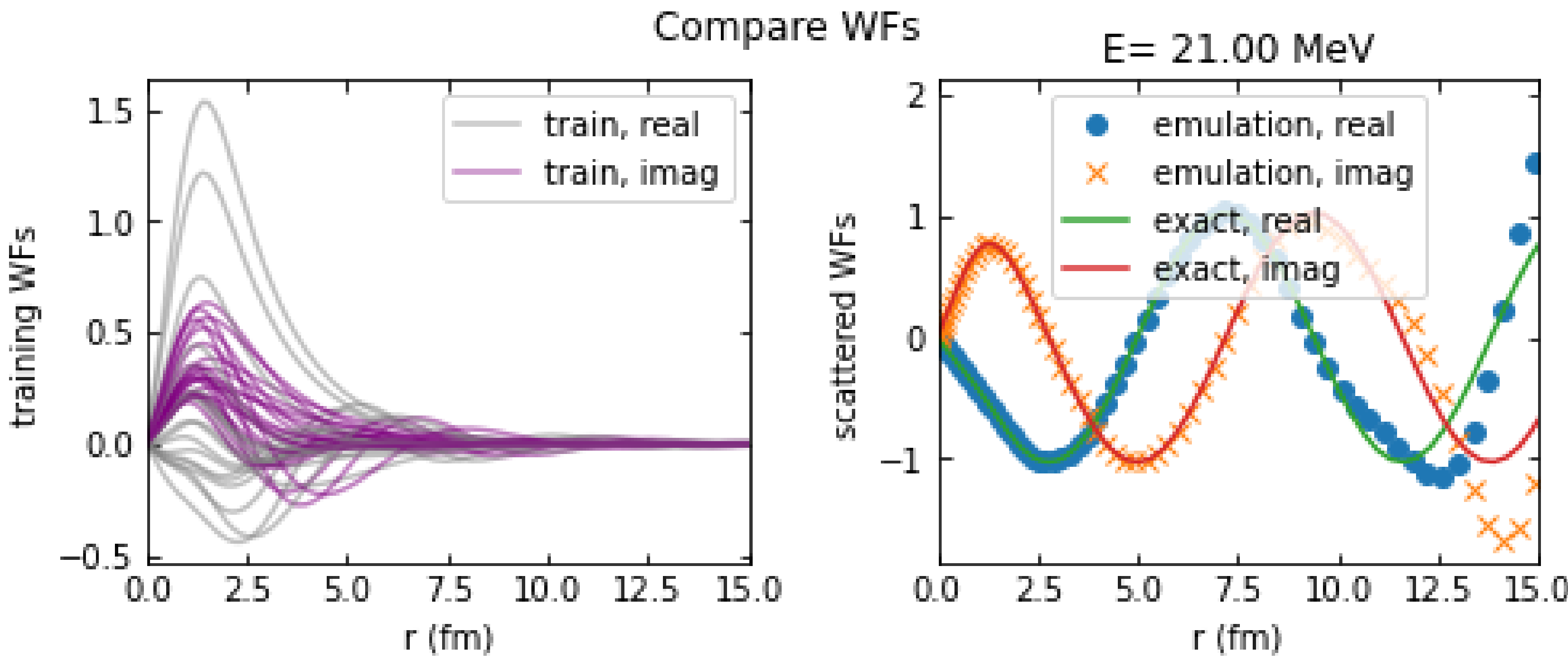
Preliminary results

Emulation in E-complex plane: two-nucleon examples

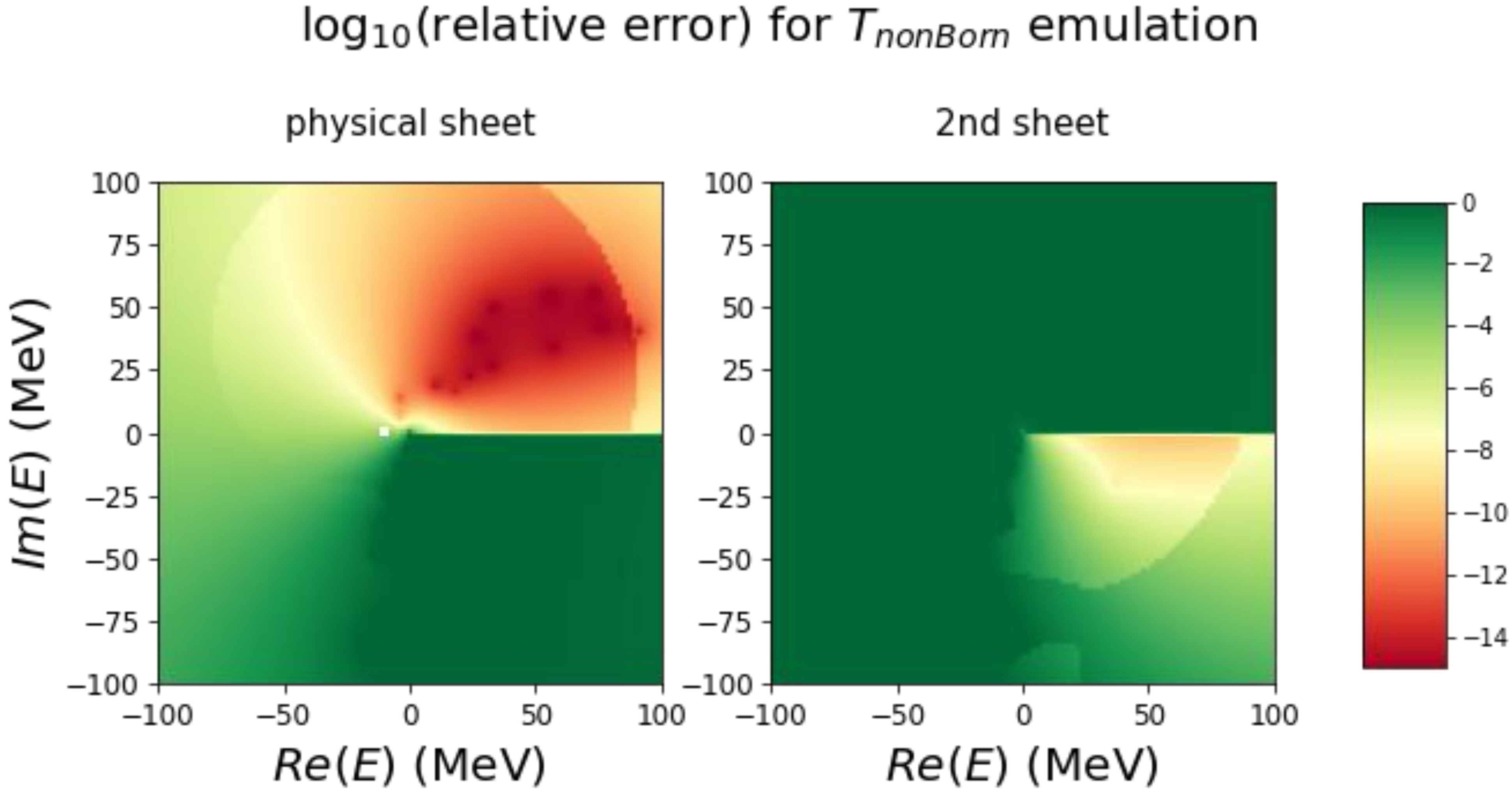
- Training wave functions (WFs) are localized
- Bound state methods for trainings



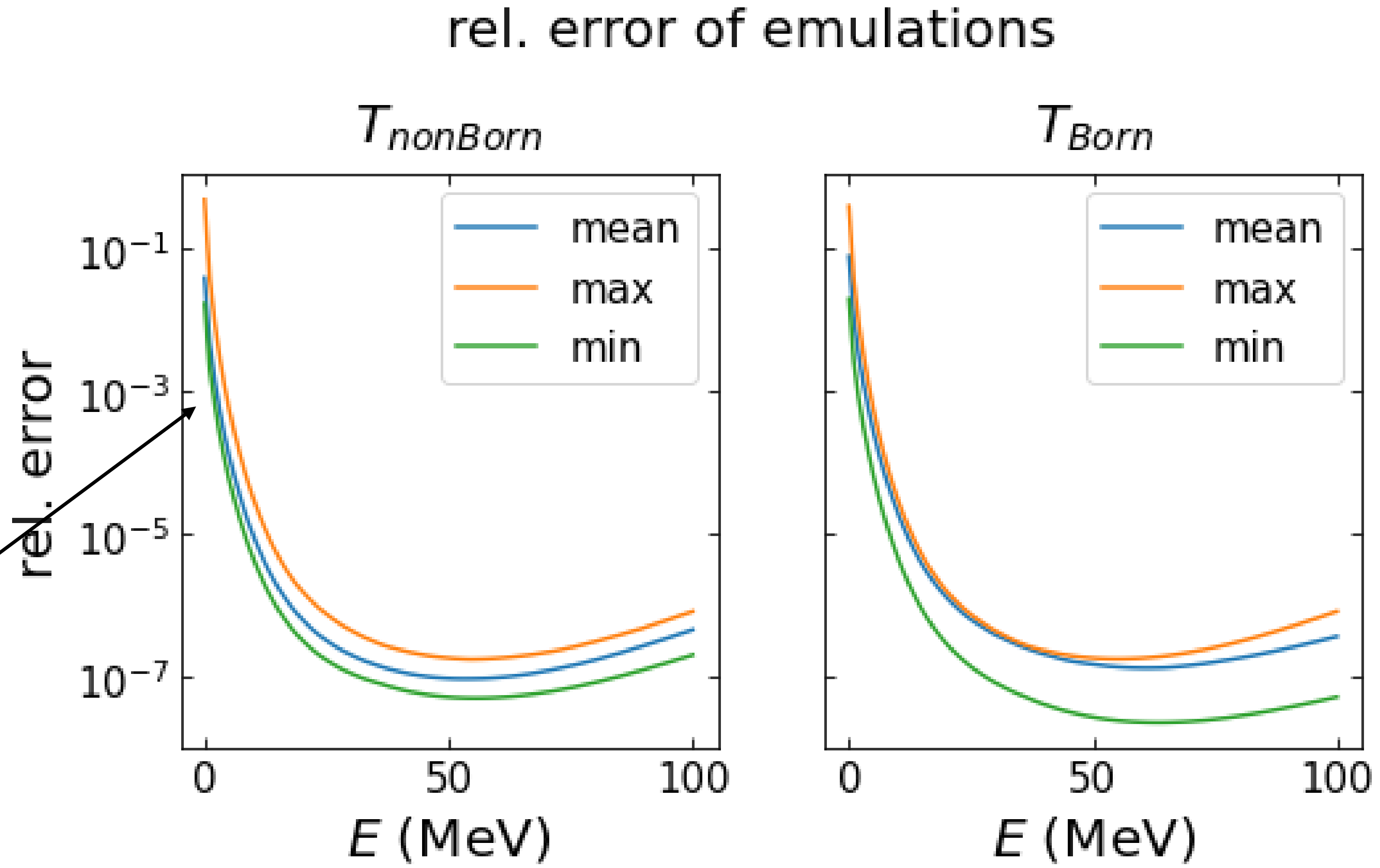
- Emulations → continuum states
- Compute continuum states based on structure solvers
- Allows emulations for other parameters



Emulation in E-complex plane: two-body in s-wave



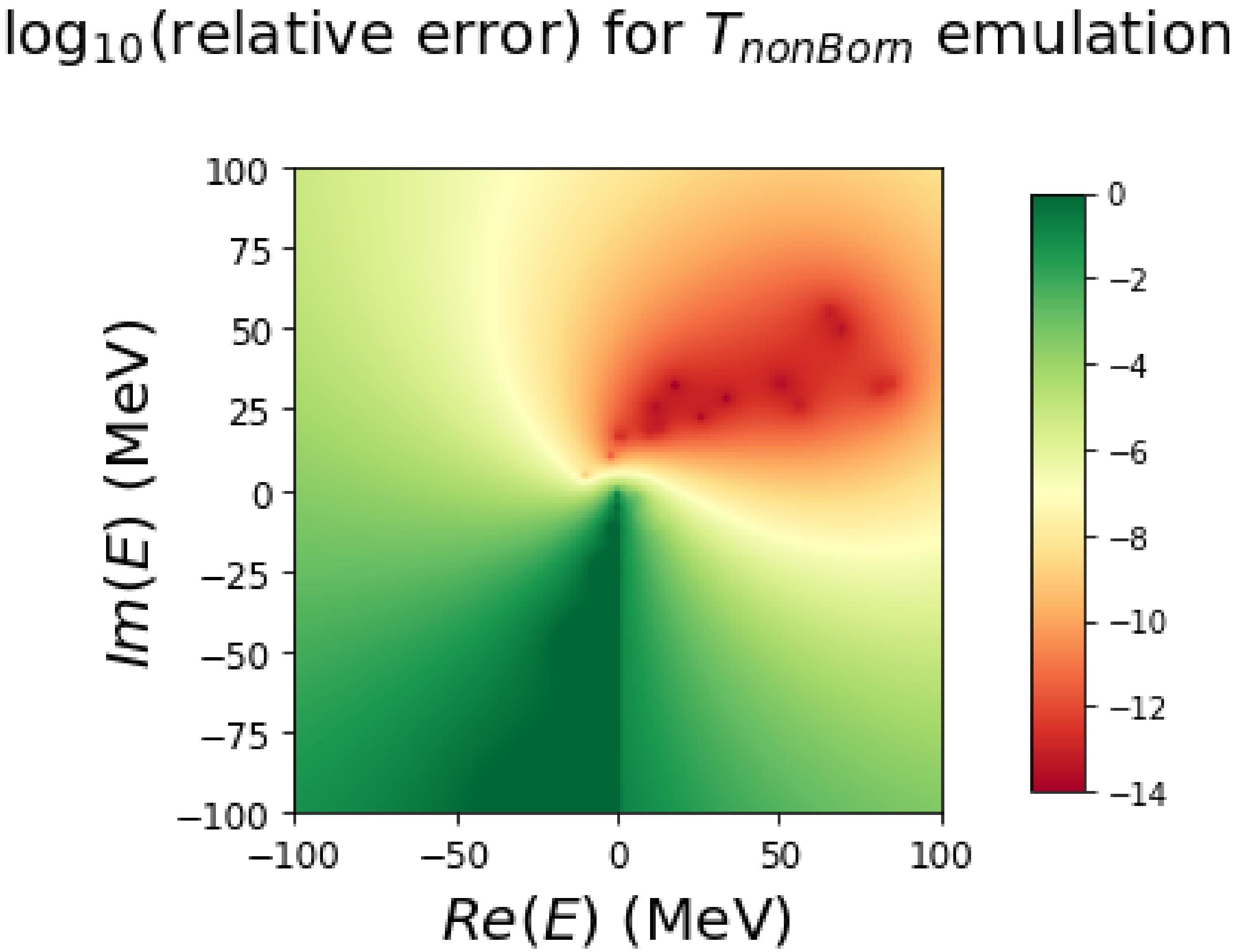
Emulation in E-complex plane: two-body in s-wave



Problematic at threshold (branch singularity)

10 training points in 4-dim space: E_{in}, $Re(E)$, $Im(E)$, potential strength

Emulation in E-complex plane: two-body in p-wave

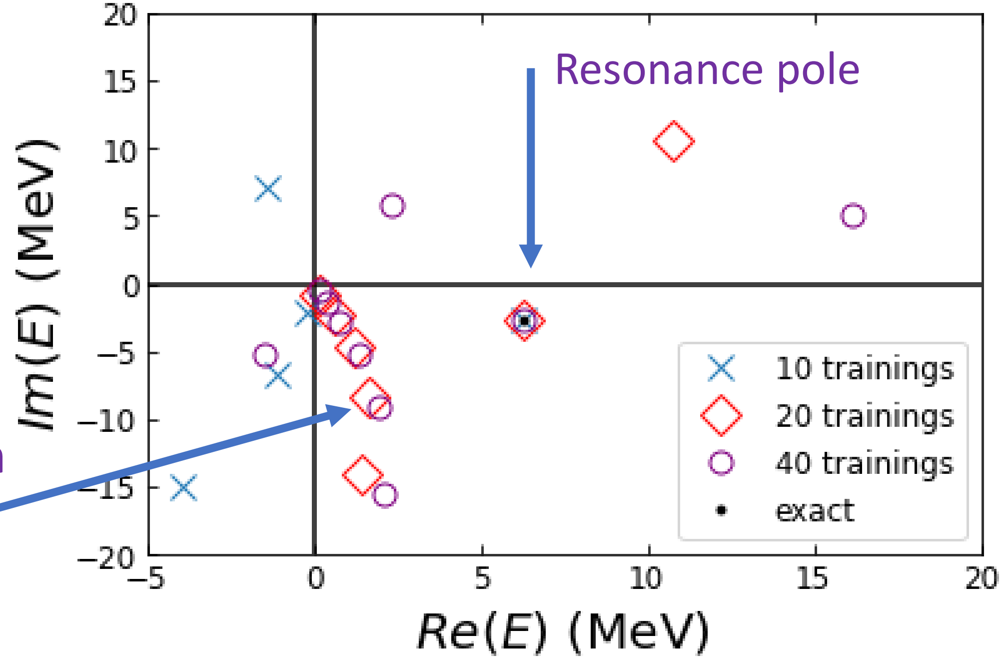


Emulation in E-complex plane: two-body in p-wave

- Emulation → fast identifications of bound state and resonances
- The pole locations are the complex eigenvalues of a complex symmetrical H (projected to training-solution subspace)

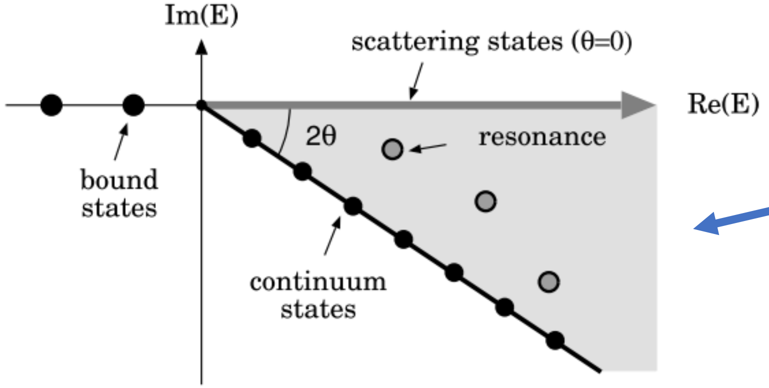
  $\langle\psi(E_i^*)|\, H|\psi(E_j)\rangle$ and $\langle\psi(E_i^*)|1|\psi(E_j)\rangle$

- Similar to other non-Hermitian approaches (complex scaling, Berggren basis) but with much smaller matrices



God's branch cut

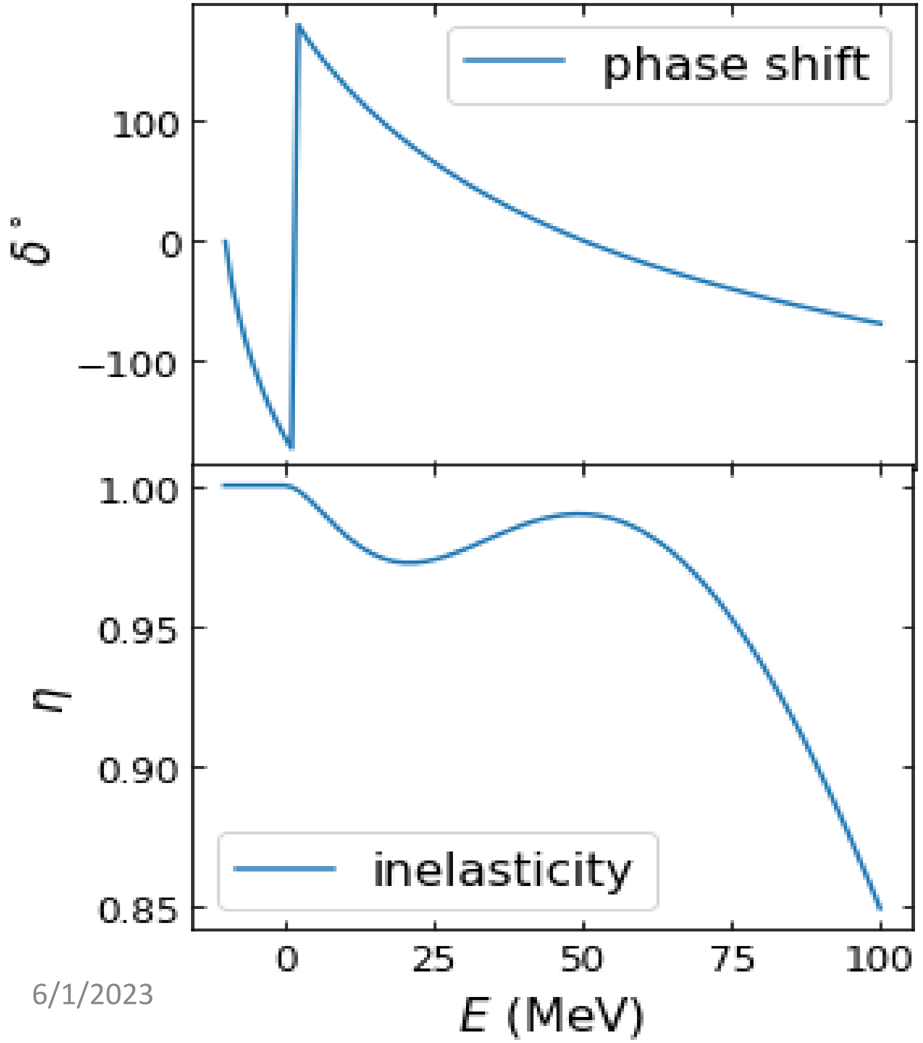
T. Myo et al. / Progress in Particle and Nuclear Physics 79 (2014) 1–56

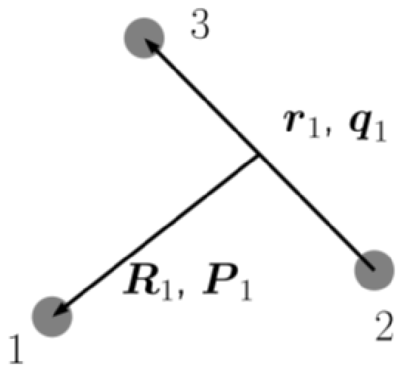


Complex scaling method

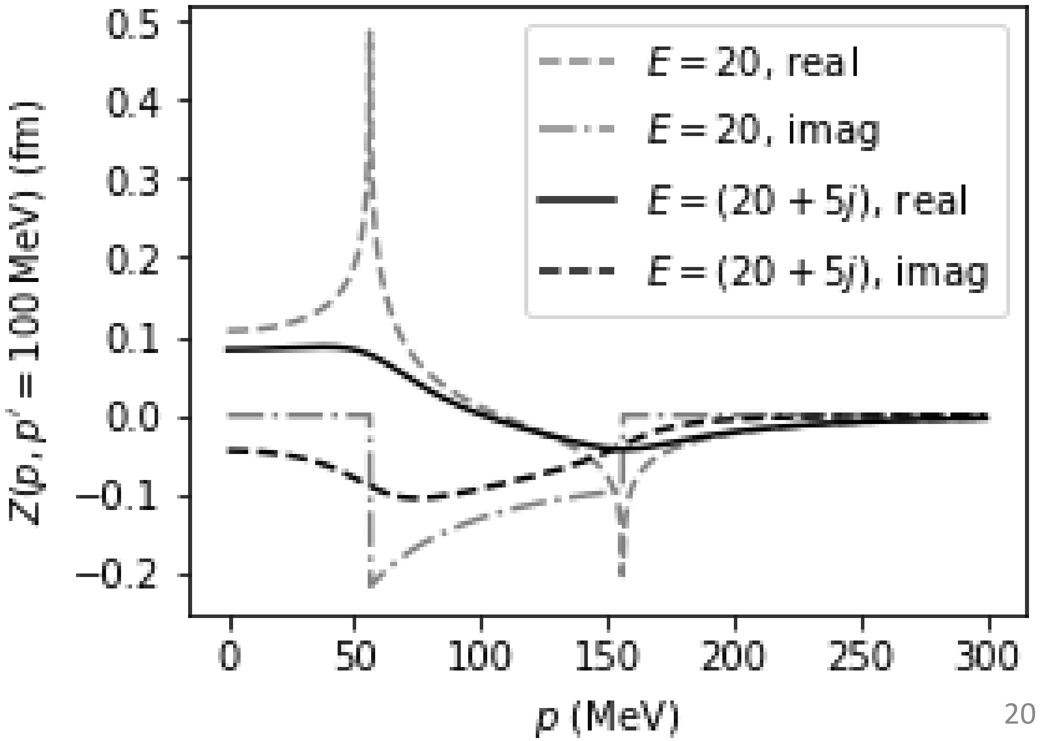
Three-boson scattering

Full calculations:



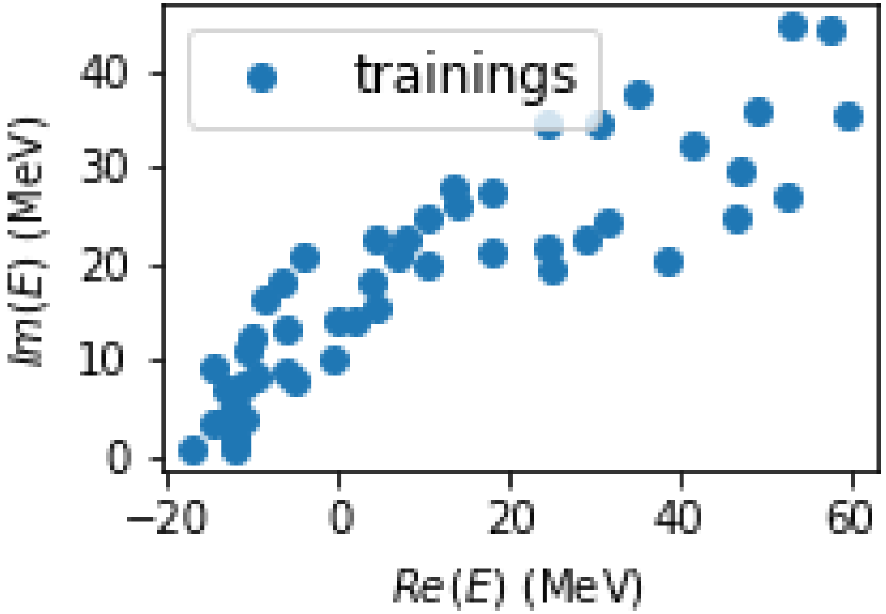


The challenge for direct continuum calculations:

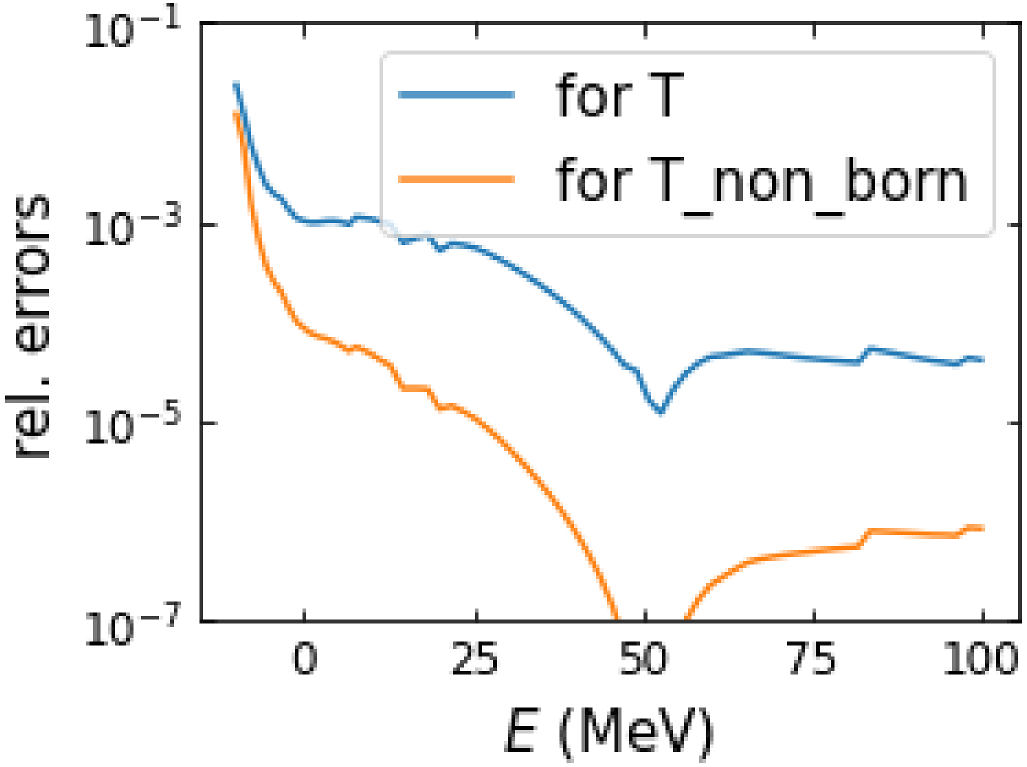


Three-boson scattering

3-dim space: $E_{in}, Re(E), Im(E)$



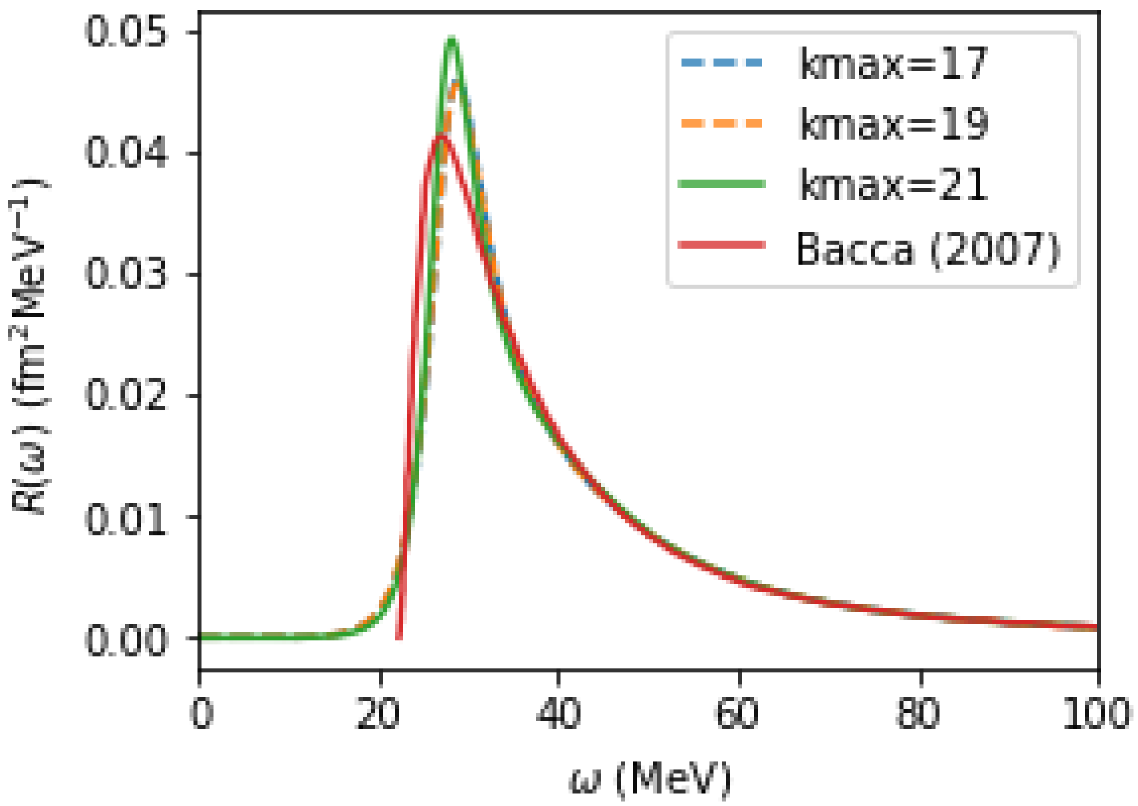
Emulation errors



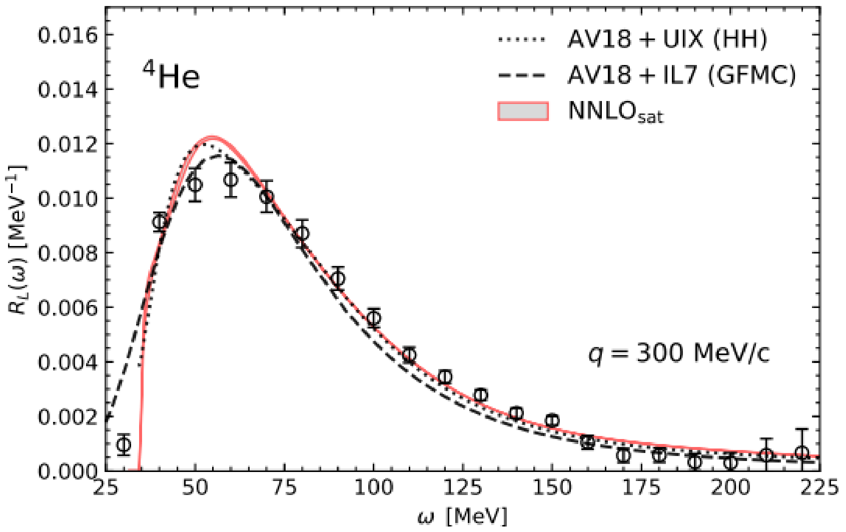
Four-body response function

With **Bijaya Acharya** and **Alex Gnech** (also experimenting with BIGSTICK, thanks to **Calvin Johnson**)

He-4 E1 response function



- Emulating for potential parameters and kinematic variables
- The near-threshold behavior is problematic (generic issue with analytical continuation on to singularities)
- It is already useful for many-body calculations



J.E. Sobczyk et. al., Phys.Rev.Lett. 127 (2021) 7, 072501 [arXiv: 2103.06786]

Comparisons to previous works

- Complex-E calculations have been performed before in few-body (scattering) and many-body (e.g., response function) calculations
- There are different methods for transferring the complex-E results to the real-energy region
  - extrapolation based on Pade approximations: started by Schlessinger&Schwartz 1966 (and their later works), and in nuclear physics by Kamada, Glockle, et. al. since 2003, later by Deltuva et. al.
  - Regression-based, such as in Lorentz integral transformation (Efros et. al. JPG: Nucl. Part. Phys. 34 R459, 2007, many works by Bacca et. al.)

$$R(\omega) = \omega^{3/2} \exp\left(-\alpha\pi(Z-1)\sqrt{\frac{2\mu}{\omega}}\right) \sum_i^N c_i e^{-\frac{\omega}{\beta i}}$$

- Complex- E emulation provides a different E-extrapolation, in addition to emulating interaction parameters and kinematic variables

Emulators for calibrating few-body models to simulations

INT Program on Nuclear Physics for Precision Nuclear Physics (April 19 to May 7, 2021).

8 Few-Body Emulators Based on Eigenvector Continuation
by Christian Drischler, Xilin Zhang

In this contribution we briefly recapitulate the progress made in constructing fast and accurate emulators for few-body scattering and reaction observables based on eigenvector continuation.[2] Emulators have been game changers and we envision them to play a key role in future workflows in nuclear physics and beyond. They have the potential to push the frontier of precision nuclear physics even further by enabling full Bayesian analyses of nuclear structure, scattering, and reaction observables, as well as by facilitating constraints for chiral interactions from (lattice) quantum chromodynamics (QCD). The future will show what other exciting applications are within reach.

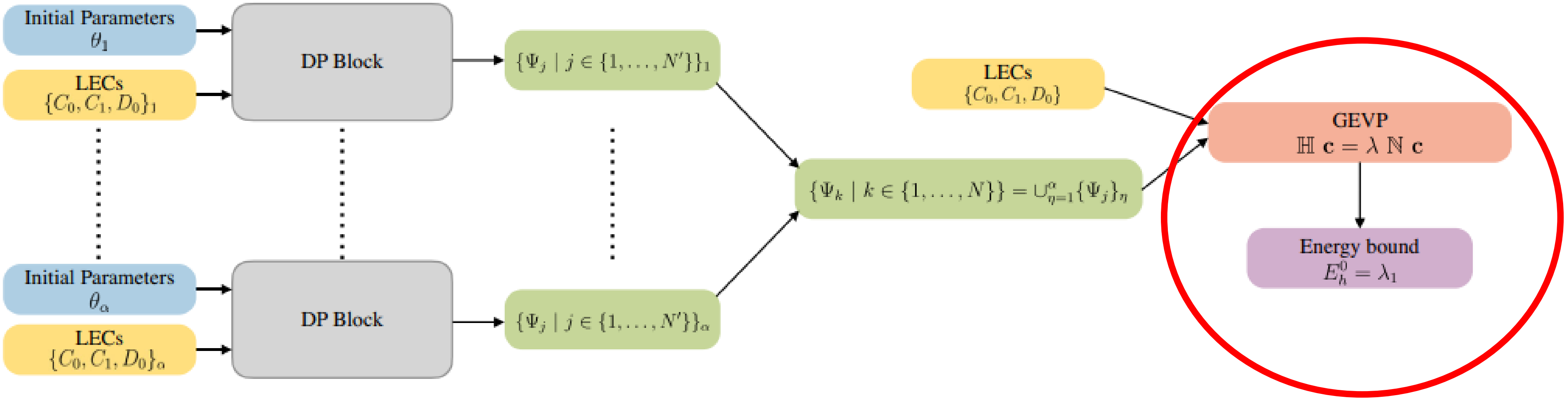
Emulators for calibrating models to simulations

PHYSICAL REVIEW D **105,** 074508 (2022)

Finite-volume pionless effective field theory for few-nucleon systems with differentiable programming

arXiv: 2202.03530

Xiangkai Sun, William Detmold, Di Luo, and Phiala E. Shanahan



(b) Generalized eigenvalue problem (GEVP) block.

Summary

- Projection-based emulators enable efficient interpolation and extrapolation for theory outputs in the input parameter space
  - They are useful for model calibration and error propagation
  - They can enable new calculations
- Real- E continuum-state emulators are being applied to realistic two and three-body calculations
- Complex- E emulators enable continuum-state calculations based on bound-state calculation methods, efficient identification of resonances, and fast interaction parameter space exploration. However, the near threshold emulations need to be improved.
- Next steps: their implementations in $N - d$ (simulation) data analysis; many-body continuum state calculations and emulations